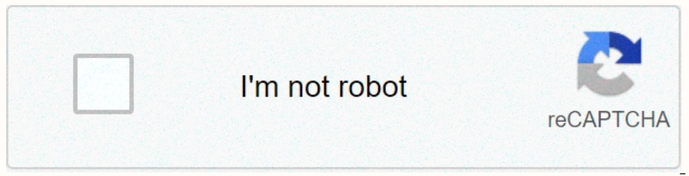

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Titration curve calculations worksheet

CurTiPot adheres to the concept of acids and bases of Brönsted and Lowry. Only the instantaneous protonation-deprotonation equilibria and the effects of ion force are calculated. No other type of chemical reaction or phase transition is taken into account in the calculations, although they may occur for many combinations of acids and bases (listed or not in the database). PH, usually measured by potentimetry with a cell comprising a glass electrode and a reference electrode, is strictly defined as -log a[H+] (see definition of pH), where a[H+] is the activity of hydrogen ions, protons more precisely hydrates, H3O+ or hydronium (the simplest type of oxanium ions). By increasing ion strength, I, ion-ionic interactions reduce the activity coefficients (gamma) of all ions including hydrated protons, H+. The pH calculator, simulation and regression modules estimate activity coefficients with the help of the Davies equation. The Davies equation gives reasonable estimates of up to approximately I ~0.1 mol/L (better than debye Hückel's equation). There are more complete equations applicable to upper I (e.g., Pitzer equation) that take into account individual hydrated ion dimension parameters and ion-ion association constants, but these are only available for a limited number of acids and bases in some electrolytes. In addition to the pH, the pH calculator also displays the p[H] and p[H]. Both correspond to -log [H+] with the difference that p[H] is calculated with thermodynamic constants but ignoring the I effect (as implodingly done in high school), while the constants used in the calculation p[H] (and also the pH) are previously corrected for effect I (ion interaction) by the Davies equation. Corrections of ion iteration are not taken into account curtipot titration and distribution modules; this does not affect the volume of the titration endpoints (stoichiometric points or equivalence points). The author provides freeware as it is, without warranties, expressed or implied, and reserves the right not to be responsible for curtipot's correctness, completeness, accuracy and error-free operation. The author did not introduce spyware, adware, viruses or malicious code into the program, as controlled and insured by many of the software's distributors (see list). Bug reports and suggestions received by email gutz@iq.usp.br. Evaluate CurTiPot freeware examples and comments CurTiPot's modular and interactive all-in-one design is intuitive and allows you to quickly calculate the pH of any watery solution, from the simplest to the most complex. The Virtual Titrator makes the simulation of the titration curve of any acid, base or mixture a breeze; flexibility in the sample size, ingredient concentration, titration range, type, size and speed of addition titration and dispersion of measurements give great realism realism The quick loading of dissociation constants and the one-click data transfer from the Virtual Titrator to both data analysis modules - Evaluation and Regression - make it easy to compare a graphical or empirical method with the numerical one in seconds! This is great for learning and teaching, as well as optimizing new titrations. Introduce the experimental volume data pairs of titration and pH readings from the pH meter (potentiometer with a combined glass electrode or other pH sensor) directly into the spreadsheet of the evaluation module. Display the curve when ing point-by-point data during lab titration or later. Select the spline bevel factor that shows the most accurate interpolation of endpoints (stoichiometric points or equivalence points) on derived curves. You will be pleasantly surprised by the effectiveness of spline sanding for volumetric titration curves with clearly defined push-ups and with the power of the regression module to deal with the most difficult data analysis. Try the regression module to get the best possible estimate of the concentrations (and pKas) of the species involved in the chemical protonation balances. The chemometric approach of the multiparametric nonlinear regression of the least squares is effective when all relevant pKas fall (or are close to the outside) of the pH range covered by the titration data. A background in chemometry, statistics or numerical data analysis is valuable but not essential to profitably explore the power and recognize the limits of the regression module, in particular, for data that cannot be treated by graphical and linearization methods (Gran plot). For example, with regression, the minimum concentrations of some acidic and basic components in strong-based titrated acid rain samples can be determined individually or grouped as follows: strong acids (H2SO4 + HNO3), weak carboxylic acid (formic + acetic), bicarbonate (H2CO3/HCO3-/CO3=) and ammonium ions (NH4+/NH3) (FORNARO, A.; GUTZ, I.G.R., Moist deposition and related atmospheric chemistry in the metropolis of São Paulo, Brazil. Part 3: Trends in precipitation chemistry during 1983-2003, Atmospheric environment, 2006, 40(30), 5893-5901). In principle, CurTiPot can simulate any titration curve in aqueous

medium regardless of the number of equilibrium acid-base mixed systems (within the above limits). The program is often downloaded by users looking for simulation and evaluation of titration curves of diprotic and triprotic amino acids. We used CurTiPot, for example, to simulate and feed pH volume values vs titration to a method of analysis of conductometric titration data (COELHO, L.H.G. and GUTZ, I.G.R., Trace analysis of acids and bases by conduction titration with nonlinear multiparametric regression, Talanta, 2006, 69(1), 204-209). The program is useful for other activities such as determining the amount of acid or base needed to neutralize a sample (neutralization), to prepare or move the pH of a swab, to change the color of a visual indicator, to find the isoelectric point of amino acids, etc. Users from one hundred and thirty countries have found freeware valuable in their research and to prepare lessons, tutorials, exercises, exam questions, laboratory guides and experiments, classroom simulations, presentations, articles, etc. Explore the multiple functions of CurTiPot now PKa database of acids and bases The user-expandable database reproduces pKa of about 250 monoprotic, diprotic and polyprotic acids and selected bases in databases of larger equilibrium constants (data references), including essential amino acids and ends with some visual indicators: acetamide, acetic acid/acetate, acetoacetic acid, acrylic/acrylate acid, adipic/adipatate acid, alanine, aminobenzene, sulphonic acid/sulfonate aminobenzene, aminophenol, ammonia, aniline, arginine, arsenic/arsenite acid, arsenate acid/arsenate, ascorbic/ascorbate acid, asparagine, aspartic/aspartate acid, barbital acid, barbiturate acid, barbiturate acid, benzenesulphonic acid, benzoic/benzoate acid, benzylamine, benzylpyridine, betaine, boric/borate acid, butanoic acid, butenoic acid, butylamine, butilammine, carbonic/carbonate acid, catechol, chloroacetic/chloroacetate acid, chloroaniline, chlorobenzoic acid, chlorophenol, choline, chromic acid, citric acid/citrate , codeine , creatinine, cynic acid, cysteine, demilammine, dichloroacetic acid, dichlorophenol, diethylamine, dimethylglylamine, dimethylpyridine, dinicotinic acid, diphenylamine, dipicolinic acid, dopamine, ephedrine, ethanolamine, ethylamine, ethylenediamine, ethylenediamine acid (EDTA), acid/formic format, fumaric acid/fumarate, glutamic acid/glutamate, glutamine, glutathione, glyceric acid, glycerol, glycine, glycolic acid, glycoxylic acid, hexaethyndiamine, hexaanoic acid, hexylamine, histamine, histidine, hydroazoic, hydrogen chloride, hydrogen chromate ions, hydrogen cian acid, hydrogen fluoride, hydrogen peroxide, hydrogen sulfide, hydrogen thiocyanate, hydroquinone, hydroxylamine, hydroxybenzoic acid, hypochlorosis, imidazole, isocytric acid, isoucine, lactic acid/lactate, ephedrine, leucine, lysine, maleic acid, malic/malate acid, malonic acid/ma melamine, methionine, methylamine, methylphenol methylpyridine, morphine, morpholine, nicotine, nitrophenol, nitrobenzoic acid, nitrous acid, norepinephrine, oxalic acid, oxaloacetic acid, poppy, pentanoic acid, perchloric/perchlorate acid, phenantroline, phenethidine , phenol, phenylacetic acid, phenylalanine, phosphate/phosphoric acid, phthalic/phthalate acid, picolinic acid, acid pylocarpin, proline, propanoic acid, propylamine, purine, pyridine, pyridinecarboxylic acid, pyrimidine, pyrimidine, pyrophosphoric acid, pyrrolidine, pyruvic/pyruvate acid, quinine, quinoline, risorcinol, saccharin, salicylic/salicylate acid, serine, silicic acid, strychnine, succinic/succinate acid, sulphuric acid/sulfate, sulfuric acid/sulphite, tartaric/tartaric acid, terephthalic/terephthalate acid, thyazole, thyoacetic acid, thyosulphonic acid, threonine, trichloroacetic acid, triethanolamine, triethylamine, triethylactic acid, tris(hydroxymethyl)-aminomethane (TRIS), tryptophan, tyrosine, urea, uric/uranus acid and valin. Examples of indicators are also included: thymol blue, methyl orange, bromocresol green, methyl red, bromotymrol blue, phenol red, phenolphtheria and alizarin yellow R. Solve acid base problems with CurTiPot Using Excel to fit a titration curve* An excel spreadsheet has been developed to help you adapt a theoretical titration curve to the pH and volume data collected in the pH titration experiment. The spreadsheet allows you to determine the end points of the titration and the pKas of the unknown acid. This document is quite long, so you can use the following hyperlinks to navigate if necessary. Quickstart The first thing to do is to download the Excel spreadsheet file acid_base_curve_fit.xls click the link. After you download the file, run Excel, open the downloaded file, and then click the tab at the bottom of the screen that indicates Differentiate. The screen should look something like the following figure. Go back to top By entering the data alert, the volume and pH data for a titration are displayed in columns A and B, respectively. The data entry columns in this spreadsheet are highlighted in green. Just click cell A2 and start entering data from the first point. After you enter each volume, press the Right Arrow key so that for the first point, for example, the active cell is B2, and then type the corresponding pH value. Then move the cursor to cell A3, click once, and enter the second reading of the volume followed by the Right Arrow key. Then enter the pH corresponding to the second volume. Move the cursor to cell A4 and continue until you have entered all the pH and volume data in columns A and B. It is very important to enter the total added base volume corresponding to each pH reading, not the buret reading. As you'll notice, Excel calculates the first and second derivatives of the curve and places them in columns E and G. The worksheet also calculates the average base volume value for each pair of points in the dataset. These values will serve as the x-axis for derived charts, the examples of which are shown below. Note you'll probably have more or less data points than you see in the sample dataset so you'll need to copy the formulas in the c-to-f columns in the cells to the right of of your data points. For example, if the data is similar to these, click the fill point in the lower-right corner of the highlighted box and drag directly down to copy formulas in C18 to G18 in rows 19 through 31, as shown below. Note that in line 31 the values are quite bizarre. This result occurs because by taking the differences, we get one less difference than the original data points. So, we could have stopped dragging to line 30. You'll also need to change the range of points to track in charts as we'll see. Go back to the top by changing the range of plot points Now moved to the part of the object that contains the titration curve, which should be similar to the one shown below. Now right-click in the white area in the edge of the chart, and the window on the left below should look as shown. Click On Source Data... to produce the window on the right above. Note that the window shows what plotting will look like when ok is clicked. In the X Values: let's see =Differentiate!$A$2:$A$30. This entry indicates that x-values will be picked from cells A2 through A30 on the Differentiation worksheet. You can change the line directly by clicking in the box, moving the cursor with the arrow keys, and deleting or adding if necessary to indicate to Excel which cells should be drawn, or by clicking the small red arrow to the right of the X Values: box, and by using the mouse to select the correct cells. Do the same thing with the Y Values box: and then click OK to produce the desired graph of the titration data. You can now print a copy of the plotted data by clicking the plot, and then clicking File/Print on the menu bar at the top of the screen. Scroll now to the area of the worksheet that contains the derived charts, as shown below. At this point, you may need to change the data selected for plotting as we did for the titration curve. Plot options are set to automatically resize the data so that the plot fills the entire space, but the options can be easily changed to enlarge any part of the path as we'll see. If you are lucky, there will be very well-defined endpoints that appear as peaks in the first derived plot and as an intersection of the curve with the x-axis in the second derived plot. Returning to the upper axis by estimating the volume of the equivalence point To find the volume of the equivalence point, we look for the point on the volume axis that corresponds to the maximum slope in the curve; that is, the first derivative should show a maximum in the Before. Now move the cursor to point directly at one of the data points on the first derived chart. A small box will appear as shown below. Note that the x (volume) and y (pH) values for the selected point appear in the box. If one of your points coincides with the apex of one or more of your peaks, you can get an estimate of your volumes of points simply by placing the cursor on the point. Take note of the approximate volumes of the equivalence points before proceeding. Now focus on the second equivalence point in the second derived curve. The calculation tells us that if the first derivative of a function passes through a maximum, the second derivative passes through zero at the same point on the x-axis. Therefore, we must find the zero crossing point on the x-axis. We will expand the horizontal scale of the chart to get a better estimate of the equivalence point, which is at the zero crossing point. It seems that the volume is about 50 mL at the second equivalence point, so we will expand the scale so that the entire x-axis covers only 4 mL and is centered on 50 mL. Your value will be different, but the principle will be identical. Now right-click the x-axis and the small window shown below will appear. To do this, you need to find an area on the axis where no data points or lines other than the axis are available. Now click Format Axis... The following window appears. Click the Minimum box: and type a number two less than the estimate of where the curve crosses the axis, which in this example is 25 mL. So, we're typing 23, so let's click in the Maximum box: and type 27. You must type the appropriate numbers for the data, and then click OK. A graph similar to the previous one therefore appears, and it should be relatively easy to estimate the volume of the equivalence point, which in the example is about 24.8 mL. Again, if one of your data is exactly at crossing point zero as one is in the chart above, you can place the cursor on the spot as shown and the point coordinates will appear in a box. Otherwise, you can estimate point by eye. Note the best estimate of the volume of the equivalence point to use on the Diprotic Acid worksheet. Go back to top By transferring data to another worksheet, Now highlight the pH data on the Differentiate as shown worksheet, and then click the Copy icon, or alternatively, you can use the menu bar and click Edit/Copy to insert the pH data on the Clipboard. Note that we did not copy cell B31 because this point is well beyond the second equivalence point. As a general rule, you don't need to use data above about 30% above the last equivalence point. In fact, it can only be beneficial to use that data up to a point just beyond the last end point, particularly if the standard base contained an appreciable amount of carbon dioxide. In our example, we estimate the second equivalence point at about 50 mL, so the at 115 mL (cell A31) is more than 100% above the second equivalence point. Then, copy the data up to 70.6 mL added. Click the Diprottic Acid tab at the bottom of the screen or the tab corresponding to the type of acid you appear to have. A should appear that looks similar to the one below. Click cell A15, and then click Edit/Paste Special... on the menu bar to reveal the window below. Click Values, and then click OK, and the pH data must be copied to column A from cell A15. You can perform the same task by typing ALT+E/ALT+S/ALT+V/ENTER. Return to the Differentiate worksheet and repeat the copy process with the volume data. Copy the data to the Diprotic Acid worksheet from cell N15 using Edit/Paste Special.../Values or by typing the sequence on the menu bar or by typing ALT+E/ALT+S/ALT+V/ENTER. Again, the data input columns have been shaded with light green to help you find the correct column. If more data is included in the dataset than the sample file, you must copy the contents of the columns B through L to include the data. Be sure to highlight the last two rows of columns B through L before clicking the fill point and copying the columns down through the last row of data. This will ensure that there is a 1 in each cell in column L. If you highlight only the last row before copying, column L is incremented when you use the fill point to copy. It is imperative that column L contains only the number 1 in each cell. Of course, if you have less data in the set than the sample set, you must delete the rows in the sample set beyond the data. Go back to top By entering other important data You must now enter several other data on the worksheet in preparation to adjust the titration curve. Note that the cells in which you need to enter data are highlighted in green, and cells that contain values calculated by Excel are highlighted in blue. First, enter the volume of the Va solution (Go into worksheet), the Veq estimate of the volume of the equivalence point from the Differentiation worksheet, and the concentration of naoh (Cb) titration from these values, Excel calculates the concentration of the unknown acid titration solution. For example, for titration of 50 mL of diprotic acid 0.1 M with 0.1 M NaOH, the spreadsheet uses the following equation. where na/nb is the number of acid moles per base mole. For the example of a diprotic acid, this ratio is 1/2. The ca value calculated in this way by Excel will be the best estimate of the acid solution concentration, but Excel may need to try to resolve this value later, particularly if the Estimate of Veq from the Differentiation worksheet is suspicious. In cell B6 (Cb), the concentration of standardized titration NaOH is in In cell B7 (Va), enter the total Volume Va of the acid titration solution. So if you followed the directions of the experiment, you pipetted 50 mL of your prepared acid solution, and then you pipetted another 50 mL of water the titration vessel. So Go into your experiment should be 100 mL. If you have not added the additional 50 mL of water, you must enter a value for Va of 50 mL. Enter a value for Veq in cell B8 (Veq); Excel will calculate and show the volume of the approximate equivalence point. The latest version of the Excel spreadsheet will automatically calculate the molar mass of the acid after you complete the curve fitting. To do this, you need to insert the mass of acid used to prepare 250 mL of the standard acid solution into cell D4. Finally, it is necessary to estimate the values for ka for acid as described in the next section. Returning to the higher estimate kas for acid, nonlinear curve fitting procedures require preliminary estimates of the parameters that will eventually be the result of the fitting process, and the Excel solver is no exception. These estimates are included in cells B1 and B2 in our example of diprotic acid. Kas for a diprotism acid can usually be estimated quite easily by the titration curve. Click the Differentiate tab and display the raw titration curve for the experiment. The curve for the sample dataset is shown below. In the sample dataset, pKa1 = 4 and pKa2 = 8, and then Ka1 = 1 ' 10-4 and Ka2 = 1 ' 10-8. Note that the points on the titration curve corresponding to pKa1 and pKa2 are circled in red. For diprotic acids that have well-separated dissociation constants and therefore well-defined equivalence points, these points correspond to the so-called semitilation points; that is, points have been added where half the number of base moles needed to reach an equivalence point has been added. Since in our example, the first equivalence point occurs at 25 mL, the titration point of the first half occurs at 12.5 mL added, which is highlighted in blue in the figure. This point on the curve corresponds to pKa1 = 4, which is shown in red next to the pH axis. The titration point of the second half occurs halfway between the first equivalence point and the second equivalence point. For the sample dataset, this point occurs at 37.5 mL of NaOH added and corresponds to pKa2 = 8, which is shown in red. If the equivalence points are well defined, you can estimate pKa1 and pKa2 as shown in the figure, calculate Ka1 and Ka2, and enter them in cells B1 and B2 on the worksheet. If the first equivalence point is not well defined, the titration curve may appear to be that of a monoprotic acid. In these circumstances, you can estimate pKa1 and pKa2 from the pH values on the curve corresponding to the titration volumes added to a quarter and three-quarters of the volume required to reach the single equivalence point The single equivalence point is determined by the Differentiate worksheet as shown above. Below is an example of this type of situation. Note that only estimates of the kas order of magnitude are necessary to obtain solver started in the corner fitting process. Thus, in this example, the two semititration points occur at 1/4 and 3/4 of the second estimated volume of the second equivalence point of 52 mL. These points at 13 mL and 39 mL correspond to pKa1 = 3 and pKa2 = 5, and Ka1 = 1 ' 10-3 and Ka2 = 1 ' 10-5, respectively. These values are then entered in cells B1 and B2 on the worksheet. It must be said at this point that if Excel is unable to obtain a solution of at least squares for the dataset and initial estimates of the kas provided, you can choose some Kas known for acids that are suspected to correspond to the unknown and use them as initial estimates. A table of dissociation constants is included in the Excel spreadsheet on the Ka's & pKa tab. Other Kas can be found in the appendices in the back of your textbook. However, to get started, you must enter the values that you determine from the dataset as shown above. Now that you have entered all experimental data and initial parameter estimates into the spreadsheet, we could proceed with the curve fitting process using the solver. Go back to top Using the Excel Solver solver function is a very powerful tool for solving equations and mounting curves. The solver uses one of several numerical methods that are similar to the method of subsequent approximations that we discussed in class. The solver allows you to select a number of options from the user, and the choice of options depends a lot on the work at hand. You may want to explore some of the solver's options after being familiar with its operation, but to begin with, we'll provide fairly specific guidance that seems to work reasonably well with titration data. This type of data is quite unusual compared to most tasks for which Excel is normally used as parameters in acid/base titrations vary over many orders of magnitude. For example, in the titration shown above, the pH varies from about 2 to about 12, which represents a change in the concentration of hydronium ions, and therefore in the concentration of hydroxide ions, of 1010. Such calculations provide an important test of the robustness and power of the Computational Engine of the Excel solver and, in general, does a magnificent job. It's important to recognize that Excel will provide answers that aren't better than the data you send them, however. To begin with, let us remember that in a least squares procedure, the aim is to find a theoretical function that adapts to the experimental data and that minimizes the sum of the squares of the residues; that is, we want to minimize the sum of squares of the differences between the experimental data and the curve On the worksheet, the sum of the residual squares is in cell B11, which is highlighted in red. When instructed correctly, the solver tries to systematically change the value values the parameters selected to find a solution that provides as few numbers as possible in cell B11. It is very important to check the summation interval in cell B11. For example, click the cell, and there should be something like =SUM(H15:H56) in the formula bar. As a general rule, you must include the data in cell B11 from the beginning of the titration up to one or two points beyond the equivalence point. For example, if the data set on this point extends to row 75, you must change the formula to B11 so that it is read =SUM(H15:H75). After you check and modify cell B11, you must ensure that all points are included in the data graph and the adapted curve. There are a couple of ways to do it. The first method starts by simply clicking on one of the curves. Some of the points will be highlighted, and rectangular boxes will appear around the x and y columns of the data being plotted. You can then click the fill point in the lower-right corner of each box and drag the rectangle to include all the data. You must repeat this process of extending the range of plot points for the mounted curve, drawn in red, and for the remaining plot. Note that you are tracing all experimental and calculated points even if you are using only points up to just beyond the equivalence point for target cell B11. Now you can recall the solver by clicking on Tools/Solver... in the menu bar, which displays the following window. Note that the target cell has been set to B11. For our purposes, the target cell is the cell containing the sum of the squares of the residues as we noted above. If you want to change the target cell, simply click the red arrow to the right of the Set Target Cell: box and select another cell. This change should not be necessary for our task. Make sure the Min button has been checked to tell the solver that we are looking for a minimum in cell B11. For other tasks, it might be advantageous to find the maximum in a numeric function or find a particular target value. Since we are running fewer squares, we want a minimum. You will also notice that it contains references to cells B1 and B2, which contain initial estimates of the dissociation constants Ka1 and Ka2. In other words, when starting the solver, it will systematically change Ka1 and Ka2 in an attempt to make the contents of cell B11 as small as possible. Now let's check the solver options to make sure they are set up correctly for our purposes. Click Options and a window appears as follows. The Maximum time: It is set for 60 seconds, which limits the amount of time the solver spends trying to minimize the minimum minimizations of the least squares. This value is much longer than is generally required. The Iterations box: is set to 100. This value limits the number of times solver calculates the sum of the squares of residues, and once again our work rarely requires this number unless something is terribly wrong. The Precision:, Tolerance:, and Convergence: boxes close the results of subsequent iterations before the solver declares the end of the process and presents the results for evaluation. These options are set to extremely small numbers. The other options and check boxes are set to ensure that the solver finds only positive solutions and that the numerical methods it uses are appropriate for our task. If you want to know more about the details of the options, click the ? When you are finished reviewing the options, click OK to return to the Solver Parameters window to start the solution process. Finally, click the Solve button to start the solver. After a few or several seconds, the following window should appear, and a new set of numbers will be produced in cells B1 and B2. At this point, you can click OK to keep the solution. In other words, Excel will replace the initial estimates with the new values for Ka1 and Ka2 in cells B1 and B2, unless you click Cancel to return to the original estimates. Typically, you click OK, assuming the results are acceptable. There are several ways to evaluate the quality of the adaptation of dissociation constants. The most obvious indicator that adaptation is acceptable is the graph of experimental data and installed data. Below is a typical example. The experimental curve is shown in black and the adapted curve is drawn in red. The texture was expanded by clicking the plot and dragging the handle into the lower-right corner. You can do the same thing with your plot to examine it more carefully. To return the plot to its original small size, you must click the cancel icon on the toolbar. Excel did a good job of mounting data in this example, but as you can see, there are deviations to high and low pH values. The fit can be improved in various ways, but a fit similar to the one shown should be enough to give you estimates of the dissociation constants that will allow you to identify acid. You can allow the solver to refine the value of Veq . To do this, return to the solver window and change the Edit Cells: box to hold the contents of cell B8 instead of the Kas value. You might also try to vary Veq and Kas at the same time. Just click the red arrow to the right of the Change Cells box: Click and drag to include the kas in cells B1 and B2, click the red arrow to the right of the Solver Parameters window. a comma, and then click the red arrow to the right of the Change Cells: Again box and select cell B8. finally click the red arrow again in the solver parameters window and then click the resolve resolve button to activate the solver. Depending on the quality of the data, you may be able to reach a global solution to the least squares process that minimizes the B11 target cell. Keep in mind that this is your ultimate goal: to minimize the sum of the residue squares in cell B11. Keep an eye on this cell as you perform the procedure of the squares more squares. The final results should be calculated and reported when the smallest possible value for cell B11 has been reached. After performing the assembly procedure, you should be sure that the results have good chemical sense. If you look at the typical values for diprotic acids in the table of dissociation constants under the Ka's & pKa tab or in Appendix 2 on the back of the textbook, you'll notice that with a few exceptions, the values range from about 10-2 to about 10-11. Values outside this range should offend chemical intuition, and you should look for errors in the solver's worksheet or options. When you are sure that you have satisfied the data in the best possible way with the Excel worksheet, you must print a copy for the records and use the results to calculate the molar mass of the acid, which along with the dissociation constants should allow you to identify the unknown acid. At this point in the session, it takes some time to play with worksheet variables. For example, change the volume value of the Veq equivalence point and note the effect on curves. Change other variables like dissociation constants and see what happens. Never underestimate the value of intellectual play. In the analysis, you can make other refinements by using task effect fixes. If you are interested in these refinements, please contact me and I will guide you through the process. In the end, I will add instructions to this document for using this feature. Back to the Top *This exercise and spreadsheet acid_base_curve_fit.xls is based on the article Titration vs . Version 1.3 27/04/98 10:42